On the completeness of the natural modes for quantum mechanical potential scattering

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On the completeness of the natural modes for quantum mechanical potential scattering

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The set of natural modes, associated with quantum mechanical scattering from a central potential of finite-range is shown to be complete. The natural modes satisfy a non-Hermitian homogeneous integral equation, or alternatively, are solutions of the time independent Schrödinger equation subject to a recently formulated nonlocal boundary condition (the quantum mechanical extinction theorem). An expansion theorem similar to that of Hilbert–Schmidt is formulated, valid for values of the solution of the scattering integral equation inside the range of the potential. The boundary conditions generated by the quantum mechanical extinction theorem are shown to be closely connected with the Jost function.

1. INTRODUCTION

For a long time attempts have been made in the theory of quantum-mechanical potential scattering to define the so-called natural modes of the scatterer. The first ones who tried to define the natural modes were Kapur and Peierls.[1] However, as it appeared to have been first pointed out by Siegert[2] their theory suffers from several unphysical phenomena like the dependence of the resonances upon the energy of the incoming wave.

Considering central symmetrical scatterers, Siegert[2] formulated another definition for the natural modes which leads to physically much more satisfactorially results. His theory was completed by Humblet and Rosenfeld.[3] An extensive survey of the literature on this subject can be found in the review article by More and Gerjoy.[4]

The definition of the natural modes given by Humblet and Rosenfeld[3] is essentially one-dimensional, because they restrict themselve to central symmetric potentials. A general definition for natural modes for quantum-mechanical potential scattering, as well as for electromagnetic scattering, has been formulated by Pattanayak and Wolf[4,5] (see also Wolf[6]). Their definition applies to genuine three-dimensional scattering problems and reduces to the Siegert–Humblet–Rosenfeld definition if the potential is central symmetric. A review of their theory, from which the basic relations of this paper are derived, is given in Sec. 2.

The natural modes can be shown to be the solutions of the radial Schrödinger equation

$$\left[-\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{l(l+1)}{r^2}+U(r)+k^2\right]\chi_l(r;k)=0\,, \tag{1.1}$$

subject to the conditions that χ_l is regular in the interval $0\leqslant r\leqslant a$, and

$$k\left[B(k)\,\chi_l(a;k)+C(k)\,\frac{\partial}{\partial a}\chi_l(a,k)\right]=0, \tag{1.2}$$

where

$$B(k)=\frac{\partial}{\partial a}\,h_l^{(1)}(ka)\,, \tag{1.3a}$$

$$C(k)=-h_l^{(1)}(ka)\,, \tag{1.3b}$$

$$U(r)=\frac{2m}{\hbar^2}\,V(r), \tag{1.3c}$$

and a denotes the range of the central symmetrical potential $V(r)$. [Siegert,[2] Humblet and Rosenfeld,[3] this paper, Sec. 2. The condition (1.2) is usually obtained from the requirement that both the field and its normal derivative are continuous across the surface of the sphere with radius a]. The purpose of this paper is to construct a Sturm–Liouville type of theory for the set of functions (natural modes) satisfying Eqs. (1.1) and (1.2) and especially to show the completeness of the natural modes inside and not *on*! the sphere with radius a. Once we have shown the completeness of the natural modes, we can solve the following initial value problem: Calculate the field inside the sphere with radius a if at $t=0$ the part of a wavepacket inside the sphere is known. To be more specific, this field can be approximated arbitrarily closely by a series

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{+l}\sum_{n}^{N}a_n(N,l,m)\;\chi_l(r,k_{ln})\,Y_l^m(\theta,\phi)\times\exp\left(i\frac{\hbar}{2m}k_{ln}^2t\right), \tag{1.4}$$

where the numbers k_{ln} are the roots of (1.2). The series $\Sigma_n^N a_n(N,l,m)\;\chi_l(r,k_{ln})$ approximates the l,mth Fourier coefficient of the initial field with respect to the set of functions $Y_l^m(\theta,\phi)$ arbitrarily closely for sufficient large N. The series only determines the field for values of $r<a$. If the boundary $r=a$ is to be included, the set of functions $\chi_l(r,k_{ln})$ is no longer complete in the interval $0\leqslant r\leqslant a$. This point will be discussed in a future paper with Dr. D.N. Pattanayak and is connected with a background scattering term.

It is unfortunately not possible to use ordinary Sturm–Liouville theory to prove the completeness of the natural modes defined by Eqs. (1.1) and (1.2) because the eigenvalue k *explicitly* shows up in the boundary condition. However, the completeness of the natural modes can be shown on using the calculus of residues. It seems that Cauchy[7] was the first one who used this method, which essentially leads to an interpolation formula, (Eq. (3.20), to prove the completeness

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of sets of functions. For similar methods and a survey of the literature we refer to Hoenders.[8]

The explicit occurrence of the eigenvalues in the boundary condition spoils the hermiticity of the problem and leads usually to nonreal eigenvalues and nonorthogonal eigenfunctions (see Morse and Feshbach[9] and Nussenzveig[10]).

It has been extensively shown in a previous publication, Hoenders,[8] that this type of problem, connected with continuity conditions on a surface, rather than boundary conditions, arises in many branches of physics. As an example, we mention the solution of an initial value problem connected with a sphere, characterized by a scalar constant complex index of refraction n_1, embedded in an infinite medium characterized by a scalar constant index of refraction n_2, in terms of the natural modes of the sphere.

The frequencies of the natural modes are determined by the continuity requirement on the tangential components of the electromagnetic field vectors which leads to an infinite set of equations similar to Eq. (1.2). Another example of a non-Hermitian problem is constructed by Morse and Feshbach.[9] They considered a string of length l which is under tension T and supported by a rigid support at $x=0$ and a nonrigid support $x=l$. This latter support has enough longitudinal strength to support the tension T, but it yields a little to transverse force imparted to it by the string. Suppose this yielding involves both friction and stiffness of the support for sidewise motion, so that the relation between the transverse force transmitted by the string, which is $-T(\partial y/\partial x)_l$, is equal to R_s times the transverse velocity of the support, $(\partial y/\partial t)_l$, plus K_s times the displacement of the support $y(l)$:

$$\begin{aligned} -T\frac{\partial y}{\partial x} &= R_s\frac{\partial y}{\partial t}+K_s y, \quad \text{at } x=l, \\ y&=0, \quad \text{at } x=0. \end{aligned} \tag{1.5}$$

If we assume that $y(x,t)=v(x)\exp(-i\omega t)$ and that $y(x,t)$ is a solution of the wave equation

$$\left(\frac{\partial^2}{\partial x^2}-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)y(x,t)=0 \tag{1.6}$$

we derive from Eqs. (1.5) and (1.6) that the functions $v_n(x)$ are the solutions of the second order linear differential equation $v_n''(x)+k_n^2 v_n(x)=0$, subject to the "boundary" conditions

$$-T\frac{\partial v}{\partial x}=-ikc\,R_s v+K_s v, \quad \text{if } x=l, \tag{1.7a}$$

$$v(0)=0, \quad \text{and} \quad \omega=ck. \tag{1.7b}$$

We cannot use the results of ordinary Sturm-Liouville theory to prove the completeness of the set of functions $\{v_n(x)\}$ because the "boundary" condition (1.7a) depends explicitly on the eigenvalue. The terminology "boundary condition" is even misleading because condition (1.7a) is not generated by a true boundary condition but arises from the condition that the force at the point 0^- is equal to the force at the point 0^+. The eigenvalues even have a nonvanishing imaginary part which accounts for the damping of the natural modes (Morse and Feshbach[9]).

It has been pointed out previously that the conditions (1.2) have been derived from a general definition for the natural modes of quantum mechanical as well as electromagnetic scattering by Wolf and Pattanayak.[5,6,11] At short survey of their theory will be given in the following Section 2, whereas the condition (1.2) will be derived in Section 3.

2. DERIVATION OF THE BASIC EQUATIONS

From the time independent Schrödinger equation

$$(\nabla^2+k^2+U(r))\psi(\mathbf{r};k)=0, \tag{2.1}$$

where

$$k^2=\frac{2mE}{\hbar^2}, \tag{2.2}$$

$$U=\frac{2m}{\hbar^2}V, \tag{2.3}$$

and with the use of Green's theorem, the following three identities can be derived:

$$\psi(\mathbf{r};k)=\int_\tau G(|\mathbf{r}-\mathbf{r}'|;k)U(\mathbf{r}')\psi(\mathbf{r}';k)d\mathbf{r}+\Sigma(\mathbf{r}), \tag{2.4}$$

$$0=\frac{1}{4\pi}[\Sigma(\mathbf{r}_<)-\Sigma^\infty(\mathbf{r}_<)], \tag{2.5}$$

$$\psi(\mathbf{r}_>)=\frac{1}{4\pi}[\Sigma^\infty(\mathbf{r}_>)-\Sigma(\mathbf{r}_>)]. \tag{2.6}$$

Here

$$\Sigma(\mathbf{r})=\iint_\sigma\left[\psi(\mathbf{r}';k)\frac{\partial}{\partial n}G(|\mathbf{r}-\mathbf{r}'|;k)-G(|\mathbf{r}-\mathbf{r}'|;k)\frac{\partial}{\partial n}\psi(\mathbf{r}';k)\right]d\sigma, \tag{2.7}$$

if

$$G(|\mathbf{r}-\mathbf{r}'|;k)=\frac{\exp(ik|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|} \tag{2.8}$$

and τ denotes a finite domain delimited by a surface σ and σ_∞ a sphere ∞ with infinite radius. All points lying inside the sphere are denoted by $\mathbf{r}_<$ and all points lying outside the sphere are denoted by $\mathbf{r}_>$.

The total wavefunction $\psi(\mathbf{r};k)$ is a superposition of the incoming wave $\psi^{(i)}(\mathbf{r};k)$ and the scattered wave $\psi^{(s)}(\mathbf{r};k)$. The latter is required to satisfy Sommerfeld's radiation condition at infinity, and therefore

$$\iint_\sigma\left[\psi^{(s)}(\mathbf{r}';k)\frac{\partial}{\partial n}G(|\mathbf{r}-\mathbf{r}'|;k)-G(|\mathbf{r}-\mathbf{r}'|;k)\frac{\partial}{\partial n}\psi^{(s)}(\mathbf{r}';k)\right]d\sigma=0. \tag{2.9}$$

Because the incoming wave satisfies Helmholtz's equation, Green's theorem yields

$$\iint_\sigma \Big[\psi^{(i)}(\mathbf{r}';k)\frac{\partial}{\partial n}G(|\mathbf{r}-\mathbf{r}'|;k)$$

$$-G(|\mathbf{r}-\mathbf{r}'|;k)\frac{\partial}{\partial n}\psi^{(i)}(\mathbf{r};k)\Big]d\sigma=\psi^{(i)}(\mathbf{r};k). \tag{2.10}$$

Combining of (2.5), (2.9), and (2.10) gives the important relation:

$$\Sigma(\mathbf{r}_< =\psi^{(i)}(\mathbf{r}_<;k), \tag{2.11}$$

which has to be satisfied for all values of $\mathbf{r}_<$ inside the sphere. Equation (2.11) is the quantum mechanical analog of the electromagnetic extinction theorem: The incoming wave is extinguished by the values of ψ and $\partial\psi/\partial n$ at the boundary. Moreover, combination of (2.4) and (2.11) leads to

$$\psi(\mathbf{r}_<)=\int_\tau G(|\mathbf{r}_<-\mathbf{r}'|,k)U(\mathbf{r}')\psi(\mathbf{r}')\,d\mathbf{r}'+\psi^{(i)}(\mathbf{r}_<), \tag{2.12}$$

which is the usual integral formulation for potential scattering for values of $\mathbf{r}$ situated inside σ. Equation (2.12) can also be shown to be valid for values of $\mathbf{r}$ situated outside σ on using the techniques of this section: Let $\mathbf{r}$ be an arbitrarily chosen point, situated outside σ and suppose that σ encloses both $\mathbf{r}$ and the scatterer. Combination of Eqs. (2.4)–(2.10) then shows the validity of (2.12) for values of $\mathbf{r}$ situated outside σ.

The natural modes for quantum mechanical scattering are defined by Wolf and Pattanayak,[4,5] as those solutions of the time independent Schrödinger equation.

$$(\nabla^2+k^2+U)\psi(\mathbf{r},k)=0, \tag{2.13}$$

satisfying the nonlocal boundary condition

$$\iint_\sigma \Big[\psi(\mathbf{r}';k)\frac{\partial}{\partial n}G(|\mathbf{r}_<-\mathbf{r}'|;k)$$

$$-G(|\mathbf{r}_<-\mathbf{r}'|;k)\frac{\partial}{\partial n}\psi(\mathbf{r}';k)\Big]d\sigma=0, \tag{2.14}$$

to be valid for all values of $\mathbf{r}_<$ lying inside σ. Hence, alternatively, Eqs. (2.4) and (2.7) show that these modes are the solutions of the homogeneus part of Eq. (2.12):

$$\psi_n(\mathbf{r}_<;k_n)=\int_\tau G(|\mathbf{r}_<-\mathbf{r}'|;k_n)\,U(\mathbf{r}')\psi(\mathbf{r}';k_n)d\mathbf{r}'. \tag{2.15}$$

It is to be stressed that the ordinary Hilbert–Schmidt theory for linear integral equations with symmetrical polar kernels cannot be used because the integral of (2.15) depends *nonlinearly* on k. The completeness of the modes (2.15) will be shown in the next section.

3. CALCULATIONAL PROCEDURE

Theorem 1: Consider the time independent Schrödinger equation

$$[\nabla^2+k^2+U(\mathbf{r})]\psi(\mathbf{r},k)=0 \tag{3.1}$$

in a spherical region of radius a bounded by a surface σ, and assume that $U(\mathbf{r})=U(r)$ is of bounded variation. Suppose that (3.1) is to be solved subject to the nonlocal boundary condition

$$\iint_\sigma \Big[\psi(\mathbf{r}';k)\frac{\partial}{\partial n}G(|\mathbf{r}-\mathbf{r}'|;k)$$

$$-G(|\mathbf{r}-\mathbf{r}'|;k)\frac{\partial}{\partial n}\psi(\mathbf{r}';k)\Big]d\sigma=0, \tag{3.2}$$

which has to be valid for *all* values of $\mathbf{r}$ lying inside the spherical region with radius a, with

$$G(|\mathbf{r}-\mathbf{r}'|;k)=\exp(ik|\mathbf{r}-\mathbf{r}'|)/|\mathbf{r}-\mathbf{r}'|. \tag{3.3}$$

Then

(1) There exists an infinite set of eigenvalues k_n and a set of eigenfunctions (natural modes) $\psi(r,\theta,\phi;k_n)$

(2) The set of natural modes is complete within the sphere of radius a.

Proof: Following the analysis given by Pattanayak and Wolf,[4] we expand the wavefunctions $\psi(\mathbf{r}_<)$ into a series of partial waves (cf. Ref. 10)

$$\psi(\mathbf{r}_<,k)=\sum_{l=0}^{\infty}\chi_l(\mathbf{r}_<,k)P_l(\cos\theta), \tag{3.4}$$

where θ is the angle between the momentum of the incoming plane wave and the direction of the vector $\mathbf{r}_<$ and the functions χ_l are the regular solutions of the radial Schrödinger equation for the l th partial wave. The expansion (3.4) and the expansion

$$G(\mathbf{r},\mathbf{r}')=k\sum_{l=0}^{\infty}(2l+1)\,j_l(kr_<)\,h_l^{(1)}(kr_>)\,P_l(\cos\theta) \tag{3.5}$$

for the Green's function (3.5), valid with $r_<=\min(|\mathbf{r}|,|\mathbf{r}'|)$ and $r_>=\max(|\mathbf{r}|,|\mathbf{r}'|)$,

where $h_l^{(1)}$ is the spherical Hankel function of the first kind and order l and Φ the angle between the directions $\mathbf{r}_<$ and $\mathbf{r}'$, are then substituted in the boundary condition (2.2), which leads to

$$\sum_{l=0}^{\infty}\alpha_l(k)j_l(kr_<)P_l(\cos\Phi)=0, \tag{3.6}$$

where

$$\alpha_l(k)=ka^2[\chi_l(a,k)h_l'^{(1)}(ka)-\chi_l'(a,k)h_l^{(1)}(ka)] \tag{3.7}$$

the prime denoting differentiation with respect to a. Because of the linear independence of the Legendre polynomials $P_l(\cos\Phi)$ in the interval $0\leqslant\Phi\leqslant\pi$ it follows that we must have $\alpha_l=0$ for all l. Equations (3.7) are a set of *local* boundary conditions imposed on the radial wavefunctions $\chi_l(r_<,k)$. From now on we will write r instead of $r_<$. For bound states and resonances states the $\alpha_l(k)$ vanish. [Pattanayak[5,6]; thus this is also true for the Jost function $L_l(k)$]. We therefore expect that both functions are closely related to each other and we will show that in accordance with this expectation both functions are proportional to each other.

The Jost function $L_l(k)$ is defined by (Newton,[12] Eq. 12.142)

$$L_l(k)=[(2l+1)!!]^{-1}k^l$$

$$\exp(-\tfrac{1}{2}i\pi l)W\{f_{l+}(k,r),\phi_l(r,k)\}, \tag{3.8}$$

where W denotes the Wronskian,

$$\phi_l(r,k)=r\chi_l(r,k), \tag{3.9}$$

f_{l+} is the solution of the Volterra equation

$$f_{l+}(k,r)=i\exp(i\pi(l-\tfrac{1}{2}))(kr)h_l^{(1)}(kr)$$

$$+\int_r^\infty G_l(r,r',k)U(r')f_{l+}(k,r')dr' \tag{3.10}$$

and

$$G_l(r,r',k)=(\cos\pi l)^{-1}\tfrac{1}{2}\pi(rr')^{1/2}$$
$$\times\{J_{l+1/2}(kr)J_{l-1/2}(kr')$$
$$-J_{l+1/2}(kr')J_{l+1/2}(kr)\}. \tag{3.11}$$

Combination of Eqs. (3.7), (3.8), and (3.9) shows that, taking $r=a$,

$$L_l(k)=(i^l)[(2l+1)!!]^{-1}k^l\alpha_l(k). \tag{3.12}$$

We will need the asymptotic expansion of $L_l(k)$ for large values of $|k|$. This asymptotic expansion is obtained on inserting the zeroth order approximation $(-1)^l(kr)h_l^{(1)}(kr)$ of $f_{l+}(k,r)$ into the integral representation, Newton,[12] §12.1,

$$L_l(k)=1+(-i)^lk^{-1}\int_0^\infty U(\tau)(k\tau)j_l(k\tau)f_{l+}(k,\tau)d\tau, \tag{3.13}$$

and replacing the spherical Bessel and Hankel functions by their asymptotic expansions. Integration by parts leads to

$$L_l(k)\sim 1+\frac{(-1)^l\exp(2ika)\,U^{(m)}(a-)}{(2ik)^{m+2}},\quad\text{if}$$
$$|k|\to\infty,\quad \pi\leqslant\arg k\leqslant 2\pi, \tag{3.14}$$

where $U^{(m)}(a-)$ denotes the first nonvanishing derivative of $U(r)$ at $r=a$, and $U^{(0)}(a-)\equiv U(a-)$, whereas the Riemann–Lebesgue theorem leads to

$$L_l(k)=1+O(k^{-1}),\quad \text{if } |k|\to\infty,\quad \pi\leqslant\arg k\leqslant 0. \tag{3.15}$$

Let the numbers λ_j be an infinite bounded set of arbitrarily chosen complex numbers. It can be shown (Hoenders,[8] Lewin[13]) that every function which is analytic inside a bounded simply connected domain D can be approximated arbitrarily closely and uniformly for all values of $k\in D$ by a suitable linear combination of a sufficiently large number of functions $\cos(\lambda_j\sqrt{k})$; i.e.,

$$(k-\delta)^{m+2}=\sum_j^n a_j(n)\cos(\lambda_jk^{1/2})+o(1), \tag{3.16}$$

if δ denotes an arbitrary complex number. Consider the contour integral

$$I_l(r,b,n)=\frac{1}{2\pi i}\int_{|k|=c_n}H(k,b)dr, \tag{3.17}$$

where

$$H(k,b)=\frac{\phi_l(r,k)\exp(ika)C(k)}{(k-\delta)^{m+2}L_l(k)(k-b)} \tag{3.18}$$

and

$$C(k)=\sum_j^n a_j(n)\cos(\lambda_j\sqrt{k}). \tag{3.19}$$

The numbers c_n are chosen in such a way that the contour passes between two successive zeros of the denominator of (3.18), and b denotes an arbitrary fixed complex number not equal to any of the zeros of $L_l(k)$. From Newton,[12] Eq. 12.137

$$\phi_l(r,k)=(2l+1)!!k^{-l-1}\sin(kr-\tfrac{1}{2}\pi l)$$
$$+o(|k|^{-l-1}\exp|\mathrm{Im}k|r),$$
$$0\leqslant\arg k\leqslant 2\pi, \tag{3.20}$$

and Eqs. (3.14), (3.15), and (3.18) we derive

$$|H(k,b)|=O\{c_n^{-1}\exp[-\tfrac{1}{2}c_n|\sin(\arg k)|(r-a)]\},$$
$$\text{if } c_n\to\infty. \tag{3.21}$$

Equations (3.17) and (3.21) lead to

$$\lim_{n\to\infty}I_l(r,b,n)=0,\quad \text{if } r<a. \tag{3.22}$$

Suppose that ρ denotes a positive number such that the domain bounded by the circle $|k-\delta|=\rho\in D$ and does not contain a zero of $L_l(k)$. These requirements can always be fulfilled by a suitable choice of the numbers ρ and δ. Calculating the integral (3.17) with the theorem of residues if $n\to\infty$ and Eq. (3.22) leads to

$$\frac{\chi_l(r,b)\exp(iba)C(b)}{(b-\delta)^{m+2}L_l(b)}$$
$$=\sum_n\frac{\chi_l(r,k_{ln})\exp(ik_{ln}a)C(k_{ln})}{L'(k_{ln})(k_{ln}-b)(k_{ln}-\delta)^{m+2}}$$
$$+\int_{|k-\delta|=\rho}H(k,b)dk, \tag{3.23}$$

if $b\neq k_{ln}$, $|b-\delta|>\rho$, and the summation has to be extended over all the zeros of $L_l(k)$. Recalling that the domain bounded by the circle $|k-\delta|=\rho$ does not contain a zero of $L_l(k)$, we derive from (3.16)

$$\left|\int_{|k-\delta|=\rho}H(k,b)dk\right|=o(1). \tag{3.24}$$

Combination of (3.23) and (3.24) yields

$$\chi_l(r,b)=L_l(b)\exp(-iba)$$

$$\times \sum_n \frac{\chi_l(r,k_{ln}) \exp(ik_{ln}a) C(k_{ln})}{L'(k_{ln})(k_{ln}-b)(k_{ln}-\delta)^{m+2}}$$

$$+o(1), \quad \text{if } b \in D \text{ and } b \neq k_{ln}. \tag{3.25}$$

While calculating the residues of the integral (3.17), we assumed that the zeros of the functions $L_l(k)$ are simple. This assumption is commonly made (Rosenfeld and Humblet,[3] Nussenzveig[10]) and is certainly true for large values of $|k|$. [Newton,[12] Eq. 12.108, gives an estimate for $L'_l(k_{ln})$ if $|k_{ln}|$ is large.] We will not analyze this difficult question but will conform with the other authors, mentioned above.

The function $\chi_l(r,k)$ is the regular solution of the radial equation

$$\left[-\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{l(l+1)}{r^2} + U(r) + k^2 \right] \chi_l(r,k) = 0. \tag{3.26}$$

Ordinary Sturm–Liouville theory shows the existence of an infinite denumerable set of eigenvalues $k_{lp}^{(1)}$ and an infinite set of eigenfunctions $\chi_l(r,k_{lp}^{(1)})$, which are regular at the origin, complete on the interval $o \leqslant r \leqslant a$, and zero if $r=a$. For every eigenvalue $k_{lp}^{(1)} \neq k_{ln}$, $n=1,2,\cdots$, we choose a simple connected domain $D \in k_{lp}^{(1)}$. Choose b to be equal to $k_{lp}^{(1)}$ in Eq. (3.20). This equation then leads to the following conclusion: Every eigenfunction $\chi_l(r,k_{lp}^{(1)})$ with $k_{lp}^{(1)} \neq k_{ln}$, $n=1,2,\cdots$, can be approximated arbitrarily closely in the interval $o \leqslant r \leqslant a$ by a suitable linear combination of functions $\chi_l(r,k_{ln})$. (If $k_{lp}^{(1)}$ would coincide with one of the numbers k_{ln}, this conclusion would be trivial!)

This conclusion proves the completeness of the set of functions $\{\chi_l(r,k_{ln})\}$ because the set of functions $\{\chi_l(r,k_{lp}^{(1)})\}$ is complete in the interval $o < r \leqslant a$. The completeness of the set of natural modes $\{\chi_l(r,k_{ln}) Y_l^m(\theta,\phi)\}$ is now easily established for any function $f(r,\theta,\phi)$ which is of bounded variation in the domain $0 \leqslant r \leqslant a$, $0 \leqslant \phi \leqslant 2\pi$, $0 < \theta < \pi$ can be expanded into the set of spherical harmonics $Y_l^m(\theta,\phi)$:

$$f(r,\theta,\phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} a_{lm}(r) Y_l^m(\theta,\phi). \tag{3.27}$$

where

$$a_{lm}(r) = \int_\Omega f(r,\theta,\phi) Y_l^m(\theta,\phi) d\Omega. \tag{3.28}$$

Because every function $a_{lm}(r)$ can be approximated arbitrarily closely by a suitable linear combination of the functions $\{\chi_l(r,k_{ln})\}$ Eq. (3.27) shows the completeness of the natural modes $\{\chi_l(r,k_{ln}) Y_l^m(\theta,\phi)\}$.

4. ON THE GENERALIZATION OF THE HILBERT–SCHMIDT EXPANSION FORMULA TO THE CASE OF KERNELS DEPENDING NONLINEARLY ON THE EIGENVALUE

In the preceeding sections we established the completeness of the natural modes $\{\chi_l(r_<,k_{ln}) Y_l^m(\theta,\phi)\}$, which are the solutions of the time independent Schrödinger equation subject to the nonlocal boundary condition (2.14). The problem, which arises immediately, in considering the linear integral equation (2.12) is the derivation of a Hilbert–Schmidt type of expansion (well-known in the theory of linear integral equations with kernels depending *linearly* upon the eigenvalue) for the unknown function. Naturally we expect that the eigensolutions of (2.12) are the most appropriate set of functions to formulate such an expansion.

By heuristical reasoning we will "derive" the desired expansion. This generalized Hilbert–Schmidt expansion explicitly shows the dependence of the expansion coefficients on k, which might be very useful for the calculation of the scattering cross section near resonances, and so provide a generalization of the Breit–Wigner formula. For recent developments connected with this expansion we refer to Hoenders[14] and Pattanayak.[15]

The expansion for the kind of problems we are analyzing was given without proof by Miranda[16] and derived by heuristical reasoning by Pattanayak.[17] We will first formulate Miranda's theorem, and then present a derivation that closely resembles the one due to Pattanayak (I am obliged to Dr. Pattanayak for making available to me his unpublished notes on this subject).

Theorem: Let the kernel function $G(x,y;\lambda)$ be defined in the square $-a \leqslant x \leqslant +a$, $-a \leqslant y \leqslant a$, symmetrical in the variables x and y, and analytic in λ. Let the function $\phi(x;\lambda)$ be the (supposedly) unique solution of the integral equation

$$\phi(x;\lambda) = f(x) + \lambda \int_{-a}^{+a} G(x,y;\lambda)\phi(y;\lambda)dy, \tag{4.1}$$

where the function $f(x)$ is defined and integrable on the interval $-a \leqslant x \leqslant +a$. If $\{\phi_n(x;\lambda_n)\}$ is the set of eigenfunctions of (4.1), satisfying the equation

$$\phi_n(x;\lambda_n) = \lambda_n \int_{-a}^{+a} G(x,\lambda;\lambda_n)\phi(y;\lambda_n)\, dy, \tag{4.2}$$

then

$$\phi(x,\lambda) = f(x) + \lambda \sum_n \left\{ \phi_n(x) \int\int_{-a}^{+a} f(y)\phi_n(y)dy \right.$$

$$\times \left[(\lambda_n - \lambda)\left(1 + \lambda_n^2 \int_{-a}^{+a} \frac{\partial}{\partial \lambda_n} \right.\right.$$

$$G(s,t)\phi_n(s)\phi_n(t)ds\,dt)]^{-1}) + \omega(x,\lambda), \tag{4.3}$$

if $\omega(x,\lambda)$ denotes a function defined on the interval $0 \leqslant x \leqslant a$ and regular in λ for all $x \in 0 \leqslant x \leqslant a$.

The formula (4.3) clearly degenerates into the well-known Hilbert–Schmidt expansion formula in case $(\partial/\partial\lambda)G(x,y,\lambda)=0$ and $\omega(x,\lambda) \equiv 0$.

Heuristic "proof": It is *assumed* that the function $\lambda^{-1}\{\phi(x;\lambda)-f(x)\}$ can be expanded into a series of partial fractions:

$$\frac{1}{\lambda}\{\phi(x;\lambda) - f(x)\} = \sum_n A_n \frac{\psi_n(x)}{\lambda - \lambda_n} + \omega(x,\lambda), \tag{4.4}$$

where $\omega(x,\lambda)$ is a regular function of λ for all values of $x \in 0 \leqslant x \leqslant a$ and $\psi_n(x)$ are functions yet to be determined. Then expanding the kernel $G(x,y,\lambda)$ into a Taylor series around the point $\lambda = \lambda_n$ up to the first order:

$$G(x,y,\lambda)$$

$$G(x,y,\lambda_n) + (\lambda - \lambda_n)\frac{\partial}{\partial \lambda_n} G(x,y,\lambda_n) + O\{(\lambda - \lambda_n)^2\}, \tag{4.5}$$

and using the identity

$$\lambda \equiv (\lambda - \lambda_n) + \lambda_n, \tag{4.6}$$

substitution of (4.4), (4.5), (4.6) into Eq. (4.1) and equating the coefficients of $(\lambda - \lambda_n)^{-1}$ and $(\lambda - \lambda_n)^0$ leads to

$$\psi_n(x) = \lambda_n \int_{-a}^{+a} G(x,y;\lambda_n)\psi_n(y)dy \tag{4.7}$$

and

$$\omega(x,\lambda_n)$$

$$= \lambda_n \int_{-a}^{+a} G(x,y;\lambda_n)\,\omega(y,\lambda_n)dy + \lambda_n$$

$$\times \int_{-a}^{+a} G(x,y;\lambda_n) f(y)\,dy$$

$$+ A_n \int_{-a}^{+a} G(x,y;\lambda_n)\,\psi_n(y)dy$$

$$+ \lambda_n A_n \int_{-a}^{+a} \frac{\partial}{\partial \lambda_n} G(x,y,\lambda)\psi_n(y)dy\,. \tag{4.8}$$

Equation (4.7) shows that the functions ψ_n are identical with the eigenfunctions $\phi_n(x)$, then, multiplying both sides of (4.8) with $\lambda_n \phi_n(x)$ and integrating over x between $-a \leqslant x \leqslant +a$, yields

$$A_n = -\lambda_n \int_a^b f(y)\,\phi_n(y)\,dy$$

$$\times \left(\int_a^b \phi_n^2(y)dy + \lambda_n^2 \right.$$

$$\left. \times \int_{-a}^{+a} \int \frac{\partial}{\partial \lambda_n} G(s,t,\lambda)\phi_n(s)\,\phi_n(t)ds\,dt \right)^{-1}. \tag{4.9}$$

On using (4.4) and (4.9) we see that (4.9) are exactly the expansion coefficients of Eq. (4.3).

It is conjectured that, as in the case of ordinary Hilbert–Schmidt theory, $\omega(x,\lambda) \equiv 0$. If this conjecture is true, combination of (3.4) and (4.3) leads to the generalized Hilbert–Schmidt expansion of (2.12):

$$\psi(\mathbf{r}_<,k) = \psi^{(i)}(\mathbf{r}_<,k) + \sum_n \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} Y_l^m(\theta,\phi) k (2l+1)$$

$$\times \frac{\chi_l(r_<,k_{ln}) \int_0^a \psi_{lm}^{(i)}(\tau) U(\tau) \chi_l(\tau,k_{ln}) d\tau}{(k_{ln} - k)(1 + k_{ln}^2 \int_0^a \int W(s,t,k_{ln}) \chi_l(s,k_{ln})}$$

$$\times \chi_l(t,k_{ln}) U(s) U(t)\,ds\,dt \tag{4.10a}$$

if

$$\psi_{lm}^{(i)}(\tau,k) = \int_\Omega d\Omega \psi^{(i)}(\tau,k) Y_l^m(\theta,\phi) \tag{4.10b}$$

and

$$W(s,t,k_{ln}) = (2l+1)\, j_l(k_{ln}s)\, h_l^{(1)}(k_{ln}t), \quad \text{if } s<t,$$

$$= (2l+1)\, j_l(k_{ln}t) h_l^{(1)}(k_{ln}s), \quad \text{if } s>t. \tag{4.10c}$$

For recent developments concerning the conjecture $\omega(x,\lambda) = 0$ we refer to Hoenders[14] and Pattanayak.[15]

DISCUSSION

The basic equations of this paper [(1.1) and (1.2)] are derived from the so-called quantum mechanical extinction theorem. This theorem is obtained by means of a procedure with which recently a *macroscopical* electromagnetic extinction theorem has been derived (Wolf[7]).

According to the Ewald–Oseen extinction theorem of molecular optics, the electromagnetic field due to an incoming wave inside a medium whose response is expressible as due to a set of dipoles can be thought of as the sum of two terms. One of these terms exactly cancels the incoming wave at every point inside the medium, and the other then gives rise to the actual macroscopical field.

The cancellation of the incoming wave is mathematically expressed by the extinction theorem (Born and Wolf[18]), the fundamental role of which for the foundations of crystal optics was already known for about 60 years from Ewald's pioneering researches, but the true meaning of which was not fully understood until very recently. During the last few years the connection between electromagnetic theory and the extinction theorem was thoroughly investigated by several authors, (Sein,[19] Wolf,[7] Pattanayak[5,6] de Goede and Mazur[20]). They all reached the conclusion that the commonly made assumption relating to the validity of this theorem for the microscopical Maxwell equations is too restrictive and that similar theorems can be derived for the macroscopic Maxwell equations as well. Wolf and Pattanayak then conjectured that the extinction theorem is to be understood as a nonlocal boundary condition to which every solution of Maxwell's equations is subjected.

In this way they completely changed the status of the extinction theorem from a *theorem* applicable only to special problems into a *principle* to be satisfied by every solution of Maxwell's equations.

The basic equations of this paper are derived from this principle. Because the complete set of functions considered in this paper is not generated by a Sturm–Liouville problem, we might expect that this set is perhaps overcomplete. This conjecture is true, as has been indicated by Humblet and Rosenfeld,[3] and a proof of this statement is given by Hoenders.[8,14]

The potential considered in this paper is rotationally symmetric, and we are therefore lead to the question if the natural modes connected with an "arbitrary" cutoff potential are also complete within the range of the potential. The completeness of such sets of natural modes has been proven by Hoenders,[14] using the inhomogeneous integral equation (2.12), with ψ^{inc} replaced by an "arbitrary" function $f(\mathbf{r})$, instead of using the Schrödinger equation (2.13) and the boundary condition (2.14).

The reason for the construction of the proof contained in this paper is that this particular technique [Eqs. (3.17), (3.22), and (3.25)] is rather simple and can be applied to similar problems which are not easily analyzed by the methods of the other proof. As an example we mention the problem of the string, discussed in the Introduction.

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